ON THE PHOTO-IONIZATION OF IMPURITY CENTRES IN SEMICONDUCTORS

M. Tomak
I. INTRODUCTION

The dependence of the photo-ionization cross-section on photon energy is mainly determined by the potential which binds the charge carrier to the impurity centre and the band structure of the host crystal. Several successful attempts have been made to calculate the photo-ionization cross-sections with the use of different impurity potentials. Lax 1) was the first to use hydrogenic theory. The characteristic feature of the hydrogen spectrum is that its maximum is at the photo-ionization threshold. Absorption then falls off with increasing photon energy. The experimental curves, however, show that peak ranges from above $E_1$ to about $2E_1$, where $E_1$ is the "observed" ionization energy 2). This discrepancy between the hydrogen model and experimental findings has motivated a number of investigators to go beyond the hydrogenic model.

Lucovsky 3) calculated the photo-ionization cross-section by using a delta-function (or zero range model) potential for the impurity. This potential describes well only the ion-core and neglects completely the long-range Coulomb effects. It is therefore expected that the model will not account for the observed cross-sections of shallower centres. As expected, Lucovsky's model agreed very well with the measured spectrum of cross-sections, in certain cases, but the agreement was not satisfactory in some other cases. A number of calculations and experiments have been performed for improving the situation and for studying the effects of electron-lattice interaction on the photo-ionization cross-section 14-17).

II. PHOTO-IONIZATION CROSS-SECTIONS

In this work, we propose yet another impurity potential model with the hope that it will do better in some physically interesting cases. The impurity potential is taken to be the Hulthen potential,

$$V(r) = -\frac{e^2}{2\alpha} \frac{e^{\alpha r/a}}{1 + e^{\alpha r/a}}.$$  

(1)

It is interesting to note that in the limit of small $r$ the Hulthen potential behaves like a Coulomb potential, whereas for large $r$ it decreases exponentially. This behaviour may be well suited for the description of screening effects. It is possible to solve the Schrödinger equation for $S_z = 0$ states. The wave function for the ground state is given by
This model potential can be used to describe shallow impurities whose spectra are well understood in terms of the effective mass approximation (EMA). In the EMA, continuum state energies are assumed to have the same distribution as that of the perfect crystal energy bands, and the corresponding wave functions are taken to be perfect crystal Bloch functions. This obviously is not applicable for deep impurities with strong, short-range potential resulting in strongly localized ground state and drastic alteration of the continuum states in the form of resonances and antiresonances.

With these restrictions in mind, the calculation of the photo-ionization cross-section is performed in two major steps. First, the wave function (2) is used as a trial function in the EMA treatment of the impurity problem where \( \lambda \) and \( a \) are treated as variation parameters to minimize the energy. Fixing \( \lambda \) and \( a \) by this procedure determines the ground state wave function completely. Then, the final state is represented by plane waves and the matrix element between the ground and final states is calculated in the electric-dipole approximation.

The photo-ionization cross-section is found to be

\[
\sigma_1(E_\text{f}) = \frac{16 \pi^2}{3} \left( \frac{\hbar \omega}{\pi} \right)^{3/2} a^2 S(E_\text{f})
\]  

where

\[
\frac{E_\text{f}}{E} = \text{the effective field ratio},
\]

\( n \) = the index of refraction,

\( \epsilon \) = the dielectric constant,

\( a = e^2/\hbar c \) the fine structure constant and

\[
S(E_\text{f}) = \frac{5}{2} a \sqrt{1 \frac{E_\text{f}}{E} - 1} \left( \frac{\hbar \omega}{\pi} \right)^{3/2}
\]

with

\[
\rho = (2m^* E_\text{f}/\hbar^2)
\]

In the case of a Yukawa type potential

\[
V(r) = -\frac{A}{e^2} \frac{e^{-r/\lambda}}{r}
\]

with the ground state wave function

\[
\psi(r) = \sqrt{\frac{2}{\pi \lambda}} \frac{e^{-r/\lambda}}{r}
\]

the photo-ionization cross-section is found to be

\[
\sigma_1(E_\text{f}) = \frac{16 \pi^2}{3} \left( \frac{\hbar \omega}{\pi} \right)^{3/2} \left( \frac{\hbar \omega}{\pi} \right)^{3/2} \left( \frac{\hbar \omega}{\pi} \right)^{3/2} \left( \frac{\hbar \omega}{\pi} \right)^{3/2}
\]

III. NUMERICAL RESULTS AND DISCUSSION

The expressions (3) and (7) can now be compared with the hydrogenic and delta function potential results: Si:P system is chosen for numerical calculations. As is well known, P is a shallow impurity in Si and the system is well studied both theoretically and experimentally. Almost all the material properties are well known. But the calculation of cross-sections requires knowledge of the quantum \( R_{\text{eff}} \) which is the effective field at the impurity site. It is extremely difficult to calculate \( R_{\text{eff}} \). The ratio \( R_{\text{eff}}/E \) has therefore generally been treated as an adjustable parameter to fix the absolute values of \( \sigma_1(E_\text{f}) \). It is clear that this factor does not affect the shape of \( \sigma(E_\text{f}) \). In this work, the ratio is taken to be approximately equal to one.

The numerical results are tabulated in Table I and are graphically displayed in Fig.1. It is encouraging to observe that the Hillen model produces the correct behaviour for the photo-ionization cross-section as a function of photon energy. The cross-section shows increased absorption at higher photon energies and displays a maximum value at about a photon energy \( \hbar \omega/E_\text{f} \approx 1.07 \). These features are rather satisfactory. The model is not expected to hold in the case of very deep impurities. In that case, from among the three main quantities that enter the calculation, namely initial and final state wave functions and the final state energies only the last can be calculated with sufficient accuracy. The accurate wave
functions are not available to make a direct prediction. As stressed by Pantelides and Jaros, one is either forced to extract a wave function from the experimental data or to use numerical wave functions which lead to a large computing effort. It is clear that more accurate calculations of bound states are necessary for accurate calculations of the photo-ionization cross-sections. The effect of electron-phonon interaction on the cross-sections, which is neglected in this work, should be taken into account especially in the case of deep impurities. Work along these lines is in progress.

ACKNOWLEDGMENTS

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste. He would also like to thank Professor I. Adawi for reading the manuscript. The support of the Scientific and Technical Research Council of Turkey is gratefully acknowledged.

REFERENCES

Table 1. Photo Ionization Cross Sections ($10^{-15}$ cm$^2$)

<table>
<thead>
<tr>
<th>$h\omega/E_x$</th>
<th>HYDROGEN</th>
<th>DELTA</th>
<th>YUKAWA</th>
<th>HÜLTHÉN</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.02</td>
<td>2.30</td>
<td>0.007</td>
<td>0.22</td>
<td>5.66</td>
</tr>
<tr>
<td>1.04</td>
<td>2.18</td>
<td>0.02</td>
<td>0.55</td>
<td>8.86</td>
</tr>
<tr>
<td>1.06</td>
<td>2.07</td>
<td>0.03</td>
<td>0.92</td>
<td>9.77</td>
</tr>
<tr>
<td>1.08</td>
<td>1.97</td>
<td>0.05</td>
<td>1.29</td>
<td>9.60</td>
</tr>
<tr>
<td>1.10</td>
<td>1.87</td>
<td>0.06</td>
<td>1.65</td>
<td>8.98</td>
</tr>
<tr>
<td>1.12</td>
<td>1.78</td>
<td>0.07</td>
<td>1.98</td>
<td>8.22</td>
</tr>
<tr>
<td>1.14</td>
<td>1.70</td>
<td>0.09</td>
<td>2.29</td>
<td>7.45</td>
</tr>
<tr>
<td>1.20</td>
<td>1.48</td>
<td>0.14</td>
<td>3.02</td>
<td>5.48</td>
</tr>
<tr>
<td>1.26</td>
<td>1.29</td>
<td>0.17</td>
<td>3.51</td>
<td>4.09</td>
</tr>
<tr>
<td>1.32</td>
<td>1.14</td>
<td>0.21</td>
<td>3.80</td>
<td>3.14</td>
</tr>
<tr>
<td>1.38</td>
<td>1.01</td>
<td>0.23</td>
<td>3.94</td>
<td>2.47</td>
</tr>
<tr>
<td>1.42</td>
<td>0.93</td>
<td>0.25</td>
<td>3.97</td>
<td>2.13</td>
</tr>
<tr>
<td>1.48</td>
<td>0.83</td>
<td>0.28</td>
<td>3.94</td>
<td>1.74</td>
</tr>
<tr>
<td>1.54</td>
<td>0.74</td>
<td>0.29</td>
<td>3.86</td>
<td>1.44</td>
</tr>
<tr>
<td>1.60</td>
<td>0.67</td>
<td>0.30</td>
<td>3.73</td>
<td>1.21</td>
</tr>
<tr>
<td>1.70</td>
<td>0.56</td>
<td>0.31</td>
<td>3.47</td>
<td>0.93</td>
</tr>
<tr>
<td>1.80</td>
<td>0.48</td>
<td>0.32</td>
<td>3.18</td>
<td>0.74</td>
</tr>
<tr>
<td>1.90</td>
<td>0.41</td>
<td>0.32</td>
<td>2.90</td>
<td>0.59</td>
</tr>
<tr>
<td>2.00</td>
<td>0.36</td>
<td>0.33</td>
<td>2.63</td>
<td>0.49</td>
</tr>
<tr>
<td>2.20</td>
<td>0.27</td>
<td>0.32</td>
<td>2.14</td>
<td>0.35</td>
</tr>
</tbody>
</table>
IC/82/114  G. LAZARIDES and Q. SHAFT - Supersymmetric GUTs and cosmology.
IC/82/115  B.K. SHARMA and M. TOMAK - Compton profiles of some 4d transition metals.
IC/82/116  M.D. HALA - Mass splitting induced by gravitation.
IC/82/117  PARTHA GHOSH - An approach to gauge hierarchy in the minimal SU(5) model of grand unification.
IC/82/118  PARTHA GHOSH - Scalar loops and the Higgs mass in the Salam-Weinberg-Glashow model.
IC/82/119  A. QADIR - The question of an upper bound on entropy.
IC/82/122  C.W. LUHG and L.Y. XIOHG - The dislocation distribution function in the plastic zone at a crack tip.
IC/82/124  BAYANT I. RAMIREZ - A view of bond formation in terms of electron momentum distributions.
IC/82/127  M.N. COHAN and M. WEIGMANN - Phasons and amplitudons in one dimensional incommensurate systems.
IC/82/128  M. TOMAK - The electron ionized donor recombination in semiconductors.
IC/82/129  S.P. TEMAMI - High temperature superconducting of a Chevrel phase ternary compound.
IC/82/130  LI XING HOU, WANG KELI and ZHANG JINGZU - Light spinor monopole.
IC/82/131  C.A. MAJID - Thermal analysis of chalcogenides glasses of the system (Ag2 Se)1-x : (Tl2 Se)x.
IC/82/133  A. QADIR - Massive neutrinos in astrophysics.
IC/82/134  H.B. GHASSIB and S. CHATTERJEE - On back flow in two and three dimensions.
IC/82/137  M.Y.M. HASSAN, A. MARIE and E.H. ISMAIL - Binding energy calculations using the molecular orbital wave function.
IC/82/138  A. BREZIN - Eigenfunctions in disordered systems near the mobility edge.
IC/82/140  Y. FUJIMOTO, K. SHIGENOTO and ZHAO ZHIYONG - No domain wall problem in SU(5) grand unified theory.
IC/82/142  S.A. CHERGOU - Trivial solution to the domain wall problem.
IC/82/143  S. CHAKRABANTI and A.K. BAYYAR - On stability of soliton solution in NLS-type general field model.
IC/82/144  S. CHAKRABANTI - The stability analysis of non-topological solitons in gauge theory and in electrodynamics.
IC/82/146  BAYANT I. RAMIREZ - Electron momentum distributions of the first-row homonuclear diatomic molecules, $A_2$.
IC/82/147  A.K. MAJUMDAR - Correlation between magnetoresistance and magnetization in Ag Rh and Au Mn spin glasses.
IC/82/149  S.A. EL WAKIL, M.T. ATIA, B.A. GHAO and A. HENDI - Particle transfer in multiregion.